UNIVERSITI SAINS MALAYSIA

Second Semester Examination
Academic Session 2007/2008

April 2008

# EKC 334 – Analysis & Operation of Catalytic Reactor
## *[Analisis Reaktor Bermangkin & Operasi]*

Duration : 3 hours
*[Masa : 3 jam]*

Please check that this examination paper consists of EIGHT pages of printed material before you begin the examination.

*[Sila pastikan bahawa kertas peperiksaan ini mengandungi LAPAN muka surat yang bercetak sebelum anda memulakan peperiksaan ini.]*

**Instructions:** Answer **FOUR** (4) questions. Answer **Question No.1** from Section A. Answer **THREE** (3) questions from Section B

***[Arahan:*** *Jawab **EMPAT** (4) soalan. Jawab **Soalan No.1** dari Bahagian A. Jawab **TIGA** (3) soalan dari Bahagian B.]*

You may answer your questions either in Bahasa Malaysia or in English.

*[Anda dibenarkan menjawab soalan sama ada dalam Bahasa Malaysia atau Bahasa Inggeris.]*

Sections A : Answer Question No. 1 is COMPULSORY.
*Bahagian A : Jawab Soalan No. 1 yang DIWAJIBKAN.*

1. [a] A non-porous spherical catalyst pellet 1 cm in diameter is suspended in a stream of liquid reactant at a suitable temperature to achieve the desired chemical reaction. The bulk concentration of the reactant is 1.0 M and its kinematic viscosity is 0.5 centistoke (1 centistoke = $10^{-6}$ $m^2/s$). For this system, the instantaneous reaction at the external surface of the pellet is known to occur at a reactant molar flux to the surface of 4.61 x $10^{-3}$ $mol/m^2$-s. By assuming the liquid diffusivity of the system is $10^{-10}$ $m^2/s$, determine the free-system liquid velocity passing through the pellet.

*Suatu pelet mangkin berbentuk sfera yang tak berliang dan berdiameter 1 sm diampaikan dalam aliran bahan tindakbalas cecair pada suatu suhu yang sesuai untuk memperolehi tindakbalas yang diinginkan. Kepekatan pukal bahan tindakbalas ialah 1.0 M dan kelikatan kinematiknya ialah 0.5 sentistoke (1 sentistok = $10^{-6}$ $m^2/s$). Bagi sistem ini, tindakbalas serta-merta pada permukaan luar pelet diketahui berlaku pada kadar fluks molar ke permukaan sebanyak 4.61 x $10^{-3}$ $mol/m^2$-s. Dengan menganggap kemeresapan cecair bagi sistem ini ialah $10^{-10}$ $m^2/s$, tentukan halaju bebas cecair yang melewati pelet tersebut.*

*[6 marks/markah]*

[b] Based on Figure Q.1. [b] that shows the diffusivity of molecules (D) in porous catalyst versus pore diameter ($d_p$), name and briefly explain characteristics of different diffusion categories as observed in the figure.

*Berdasarkan Rajah S.1. [b] yang menunjukkan kemeresapan molekul (D) dalam mangkin berliang melawan diameter liang ($d_p$), namakan dan terangkan dengan ringkas ciri-ciri berbagai kategori resapan sebagaimana yang ditunjukkan oleh rajah tersebut.*

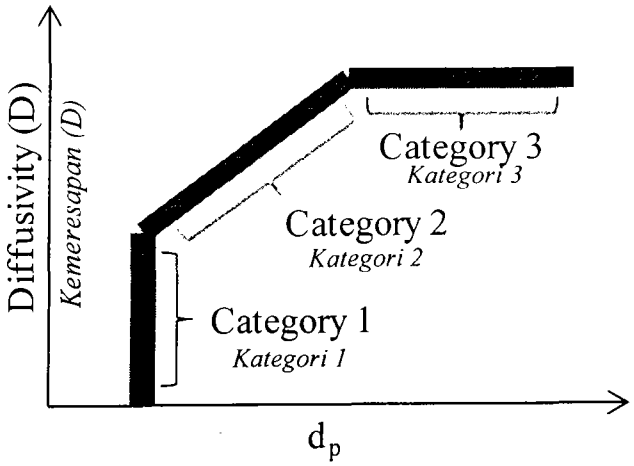


Figure Q.1. [b]
*Rajah S.1. [b]*

*[6 marks/markah]*

...3/-

[c] For an isothermal particle of "flat-plate" geometry (at the surrounding bulk-gas temperature) of species B reacting with gaseous species A, derive a relationship to determine the time t required to reach a fraction of B converted ($X_B$) according to the Shrinking Core Model (SCM), if the chemical reaction is controlling. The reaction is a first-order surface reaction. State any assumptions.

*Bagi sebutir zarahan sesuhu spesis B dengan geometri plat rata (pada suhu gas pukal sekitaran) yang bertindakbalas dengan spesis gas A, terbitkan suatu hubungan yang akan menentukan masa t yang diperlukan untuk mencapai pecahan penukaran B ($X_B$) menurut Model Teras Mengecut (SCM). Proses ini dikawal oleh tindakbalas kimia. Tindakbalas tersebut ialah suatu tindakbalas permukaan tertib pertama. Nyatakan sebarang andaian yang dibuat.*

*[13 marks/markah]*

Sections B : Answer any THREE questions.
*Bahagian B : Jawab mana-mana TIGA soalan.*

2. [a] Discuss the importance of chemisorption in a chemical reaction.

*Bincangkan kepentingan jerapan kimia dalam sesuatu tindakabalas kimia.*

*[6 marks/markah]*

[b] Given in Figure Q.2. [b] is the generalized diagram of turnover frequency (TOF) versus reaction temperature for various industrial reactions. Provide an analysis of the figure on the basis of the occurrence of chemisorption, energy barrier and reaction rate.

*Rajah S.2. [b] menunjukkan gambarajah umum frekuensi pusingan balik (TOF) melawan suhu tindakbalas bagi berbagai tindakbalas industri. Berikan analisis rajah tersebut berdasarkan kejadian jerapan kimia, halangan tenaga dan kadar tindakbalas.*

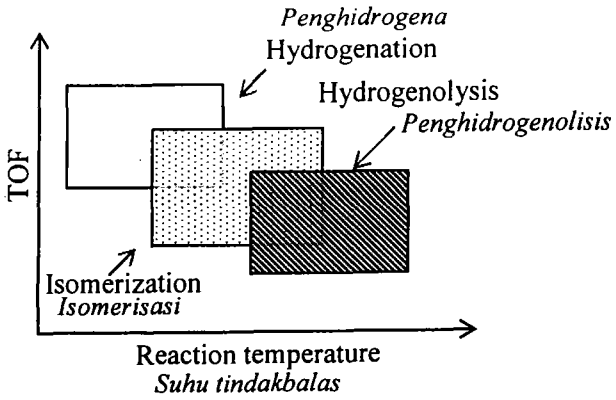


Figure Q.2. [b]
*Rajah S.2. [b]*

*[8 marks/markah]*

[c] The reaction between propionaldehyde (A) and hydrogen ($H_2$) to form propanol (B) is catalyzed by a supported catalyst. In a differential reactor experiment, the reaction rate can be related to the partial pressure of the reactants by,

$$-r_A' \frac{P_A}{P_{H_2}^{0.5}}$$

By assuming dissociative adsorption of hydrogen on the active site of the catalyst and the rate limiting step is the adsorption of A, determine whether this expression is more applicable to high or low partial pressure of hydrogen.

*Tindakbalas antara propionaldehid (A) dan hidrogen ($H_2$) bagi membentuk propanol (B) dimangkinkan oleh suatu mangkin bersokongan. Dalam suatu ujikaji reaktor kebezaan, kadar tindakbalas boleh dihubungkan dengan tekanan separa bahan-bahan tindakbalas,*

$$-r_A' \frac{P_A}{P_{H_2}^{0.5}}$$

*Dengan menganggap penjerapan tercerai hidrogen pada tapak aktif mangkin dan peringkat pengawal kadar ialah proses penjerapan A, tentukan samada hubungan ini lebih sesuai kepada tekanan separa hidrogen yang rendah atau tinggi.*

*[11 marks/markah]*

3. [a] An integral reactor packed with different amounts of porous catalyst is used to determine the rate expression of a chemical reaction represented as,

*Suatu reaktor kamiran yang diisi dengan amaun mangkin berliang yang berlainan digunakan untuk menentukan hubungan kadar bagi tindakbalas kimia yang diwakili sebagai,*

$$A \rightarrow 4R$$

The molar flow rate of the reactant charged into the reactor is fixed at 10 mol/h with an initial concentration of 0.1 mol/l. Data collected are tabulated as given in Table Q.3. [a].

*Kadar alir molar bahan tindakbalas ke reaktor itu ditetapkan pada 10 mol/jam pada kepekatan permulaan sebanyak 0.1 mol/l. Data yang dikumpulkan telah diberikan dalam Jadual S.3. [a].*

Table Q.3.[a]
*Jadual S.3.[a]*

| W, kg of catalyst *W, kg mangkin* | 1 | 2 | 3 | 4 | 5 | 6 | 7 |
|---|---|---|---|---|---|---|---|
| $X_A$ | 0.12 | 0.20 | 0.27 | 0.33 | 0.37 | 0.41 | 0.44 |

Determine the rate expression for this reaction.
*Tentukan hubungan kadar bagi tindakbalas ini.*

*[11 marks/markah]*

...5/-

[b] With the help of a suitable diagram, discuss the profiles of reaction concentration around and within a porous catalyst pellet for cases of reaction control, external mass transfer control and pore diffusion control.

*Dengan berbantukan rajah yang sesuai, bincangkan profil-profil kepekatan bahan tindakbalas disekitar dan di dalam suatu pelet mangkin berliang bagi kes-kes kawalan tindakbalas, kawalan pemindahan jisim luaran dan kawalan peresapan liang.*

*[6 marks/markah]*

[c] Discuss the common problems that are likely to be encountered when conducting a differential reactor experiment to determine the reaction rate for a solid catalyzed reaction.

*Bincangkan masalah-masalah biasa yang mungkin dialami bila melakukan ujikaji reaktor kebezaan bagi penentuan kadar tindakbals bagi suatu tindakbalas bermangkinkan pepejal*

*[8 marks/markah]*

4. [a] Solid particles containing B are roasted isothermally in an oven with gas of constant composition. The solids are converted to a firm nonflaking product according to Shrinking Core Model (SCM) as follows:

*Zarah-zarah pepejal yang mengandungi B dipanggang secara sesuhu dalam sebuah ketuhar dengan gas berkomposisi malar. Pepejal tersebut ditukarkan ke suatu produk kukuh tak berkelupas menurut Model Teras Mengecut (SCM) seperti yang berikut:*

$$A(g) + B(s) \rightarrow R(g) + S(s)$$

The following data are available:

*Data berikut telah diperolehi:*

| $D_p$, mm | $X_B$ | $t$, min |
|---|---|---|
| 1 | 1 | 3.3 |
| 1.5 | 1 | 7.50 |

$C_A = 0.010$ kmol/m$^3$ , $\rho_B = 20$ kmol/m$^3$

Determine the rate controlling mechanism for the transformation of solid.

*Tentukan mekanisma pengawalan kadar bagi transformasi pepejal.*

*[17 marks/markah]*

[b] Complete the following statements:

*Lengkapkan kenyataan-kenyataan berikut:*

[i] A typical heterogeneous catalyst is comprised of three components:

*Suatu mangkin heterogen lazim mengandungi tiga komponen:*

(a) ..... (b) ..... (c) .....

[ii] Mechanical properties of catalysts include:

*Sifat-sifat mekanik mangkin termasuk:*

(a) ..... (b) .....

[iii] Micropore volume is .....
*Isipadu mikroliang ialah* .....

[iv] Crystallinity is .....
*Kehabluran ialah* .....

[v] A BET (Brunauer, Emmett and Teller Method) is .....
*Kaedah Brunauer, Emmett dan Teller (BET) ialah* .....

[vi] Infrared (IR) spectroscopy can be used to:
*Spektroskopi inframerah (IR) boleh digunakan untuk:*

(a) ..... (b) .....

[vii] In a gas-solid reaction, the film resistance at the surface of a particle is dependent on many factors such as:
*Dalam tindakbalas gas-pepejal, rintangan saput di permukaan suatu zarah bergantung kepada banyak faktor seperti:*

(a) ..... (b) ..... (c) .....

[viii] Three factors that control the design of a fluid-solid reactor:
*Tiga faktor mengawal rekabentuk reaktor bendalir-pepejal:*

(a) ..... (b) ..... (c) .....

*[8 marks/markah]*

5. [a] Iron sulfide particles dispersed in asbestos fibers are roasted and the particles remained as hard solids of unchanging size during reaction. A fluidized-bed reactor is planned to convert the particles to the corresponding oxide. The feed is to be uniform in size, $\tau$ = 20 min, with mean residence time $\bar{t} = 60$ min in the reactor. Find the fraction of original sulfide ore remaining unconverted if the time for complete conversion is related to particle size as follows:

[i] $\tau \alpha R$
[ii] $\tau \alpha R^2$
[iii] Comments on your results

**State your assumptions.**

*Zarah-zarah besi sulfida yang terserak dalam gentian asbestos telah dipanggang dan zarah-zarah tersebut kekal sebagai pepejal keras yang tidak bertukar saiz semasa tindakbalas. Suatu reaktor lapisan terbendalir telah dirancang untuk menukarkan zarah-zarah tersebut kepada oksida yang sepadan. Suapan adalah bersaiz seragam,* $\tau$ = *20 min, dengan masa mastautin ialah* $\bar{t} = 60$ min *dalam reaktor. Carikan pecahan bijih sulfida asal yang masih kekal tak bertukar jika masa untuk penukaran penuh mempunyai hubungan dengan saiz zarah seperti yang berikut:*

*[i]* $\tau \alpha R$
*[ii]* $\tau \alpha R^2$
*[iii] Komen keputusan anda*

***Nyatakan andaian anda.***

*[15 marks/markah]*

...7/-

[b] Answer the following questions **true** or **false**:
*Jawab benar atau palsu bagi soalan-soalan berikut:*

[i] Acidity in zeolites increases with a decreasing Si:Al.
*Keasidan zeolit meningkat dengan penurunan Si:Al.*

[ii] In plug flow reactor, all solids stay in the reactor for the same length of time.
*Dalam reaktor aliran palam, kesemua pepejal berada dalam reaktor untuk tempoh masa yang sama.*

[iii] Sulfiding treatment is the first step in the production of sulfide catalysts.
*Rawatan pensulfidaan ialah langkah pertama dalam pengeluaran mangkin sulfida.*

[iv] X-ray diffraction (XRD) is a powerful tool for examining the role of adsorption steps in catalysis.
*Pembelauan sinar-X (XRD) ialah suatu alat yang berkesan untuk menguji peranan langkah-langkah penjerapan dalam pemangkinan.*

[v] Transition electron microscopy (TEM) is a useful tool for determining crystallite size and size distribution for supported metals.
*Mikroskopi elektron teralih (TEM) ialah suatu alat yang berkesan untuk menentukan saiz kristalit dan taburan saiz logam tersokong.*

[vi] Impregnation by incipient wetness is usually applied to pelletized supports.
*Pengisian melalui kebasahan awal biasanya digunakan untuk penyokong teruntil.*

[vii] Thermogravimetric (TG) is specifically investigating a change in sample mass as a function of pressure.
*Termogravimetri (TG) menyiasat secara khusus perubahan jisim sampel sebagai suatu fungsi tekanan.*

[viii] The operation of a Differential Scanning Calorimeter (DSC) is based on measurement of the thermal response of an unknown specimen as compare with a standard when the two are heated uniformly at a constant rate.
*Operasi sebuah kalorimeter pengimbasan pembezaan (DSC) adalah berdasarkan pengukuran sambutan terma bagi suatu spesimen yang tidak diketahui berbanding dengan suatu piawai apabila kedua-duanya dipanaskan secara seragam pada kadar malar.*

[ix] According to Shrinking Core Model, reaction occurs first at the outer skin of the particle. The zone of reaction then moves into the solid, leaving behind completely unconverted material and inert solid.

*Menurut Model Teras Mengecut, tindakbalas mula-mula berlaku di kulit luar zarah tersebut. Zon tindakbalas kemudiannya bergerak ke dalam pepejal dan meninggalkan bahan tak tertukar penuh serta pepejal lengai.*

[x] When hard product material is formed during a reaction, ash layer diffusion can be ruled out as the controlling resistance.

*Apabila bahan produk keras terbentuk semasa suatu tindakbalas, resapan lapisan abu boleh diketepikan sebagai rintangan pengawal.*

*[10 marks/markah]*

- ooo O ooo -